

#Ligand	TotalEnergy	VDW	AverConPair
6m2q-Roccustyrna_fr1-0.pdb	-896.465	-896.465	10.058
6m2q-Roccustyrna_fr2-0.pdb	-798.627	-798.627	165.152
6m2q-Roccustyrna_fr3-0.pdb	168.424	168.424	134.359
6m2q-Roccustyrna_fr4-0.pdb	-785.438	-785.438	151.111
6m2q-Roccustyrna_fr5-0.pdb	348.743	348.743	794.118
6m2q-Roccustyrna_fr6-0.pdb	-904.774	-904.774	173.421
6m2q-Roccustyrna_fr7-0.pdb	-846.778	-846.778	210.286
6m2q-Zanamivir_CID_60855-0.pdb	-613.535	-613.535	166.522
6m2q-Vidarabine_CID_21704-0.pdb	-661.163	-661.163	230.526
6m2q-Valganciclovir_CID_135413535-0.pdb	198.156	198.156	22.84
6m2q-Tenofovir_CID_464205-0.pdb	-638.549	-638.549	215.789
6m2q-Taribavirin_CID_451448-0.pdb	-606.346	-606.346	222.353
6m2q-Sorivudine_CID_5282192-0.pdb	820.449	820.449	18.05
6m2q-Sofosbuvir_CID_45375808-0.pdb	296.684	296.684	188.056
6m2q-Ritonavir_CID_392622-0.pdb	155.543	155.543	8.8
6m2q-Penciclovir_CID_135398748-0.pdb	-69.663	-69.663	251.111
6m2q-Nelfinavir_CID_64143-0.pdb	487.507	487.507	25.95
6m2q-Merimepodib_CID_153241-0.pdb	-821.219	-821.219	160.606
6m2q-Maribavir_CID_471161-0.pdb	-720.599	-720.599	204.167
6m2q-Lopinavir_CID_92727-0.pdb	353.779	353.779	178.261
6m2q-Indinavir_CID_5362440-0.pdb	-920.937	-920.937	184.889
6m2q-Inarigivir_CID_6912016-0.pdb	-904.684	-904.684	144.359
6m2q-Galidesivir_CID_10445549-0.pdb	-700.417	-700.417	221.579
6m2q-Famciclovir_CID_3324-0.pdb	484.732	484.732	217.391
6m2q-Faldaprevir_CID_42601552-0.pdb	196.047	196.047	150.175
6m2q-Darunavir_CID_213039-0.pdb	-811.094	-811.094	134.211
6m2q-Cytarabine_CID_6253-0.pdb	-590.168	-590.168	223.529
6m2q-Boceprevir_CID_10324367-0.pdb	242.807	242.807	15
6m2q-Atazanavir_CID_148192-0.pdb	290.66	290.66	193.137
6m2q-Asunaprevir_CID_16076883-0.pdb	-797.693	-797.693	133.529
6m2q-Amprenavir_CID_65016-0.pdb	-813.987	-813.987	162.571
6m2q-GissitorviffirnaTM1-0.pdb	-70.081	-70.081	216.818
6m2q-GissitorviffirnaTM4-0.pdb	-69.95	-69.95	22.8
6m2q-GissitorviffirnaTM6-0.pdb	166.473	166.473	140.256
6m2q-GissitorviffirnaTM7-0.pdb	-790.107	-790.107	135.789
6m2q-GissitorviffirnaTM8-0.pdb	-731.542	-731.542	154.737
6m2q-GissitorviffirnaTM9-0.pdb	-842.045	-842.045	187.353
6m2q-Roccustyrna_gs1-0.pdb	261.182	261.182	138.043
6m2q-Roccustyrna_gs2-0.pdb	-690.297	-690.297	235.263
6m2q-Roccustyrna_gs3-0.pdb	204.639	204.639	182.766
6m2q-Roccustyrna_gs4-0.pdb	-334.177	-334.177	898.039
6m2q-Roccustyrna_gs5-0.pdb	100.983	100.983	10.5
6m2q-Roccustyrna_gs6-0.pdb	-635.585	-635.585	24
6m2q-Roccustyrna_gs8-0.pdb	306.373	306.373	12.74